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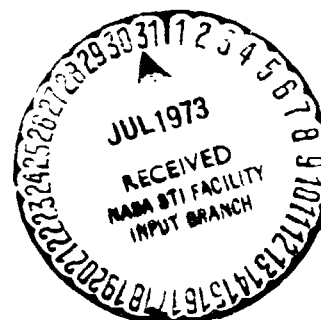
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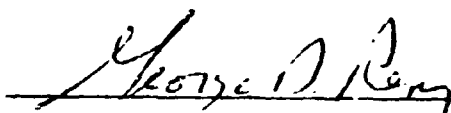
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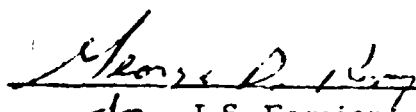
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FOREWORD

This document presents the results of work performed by the Fluid Mechanics Section of the Aeromechanics Department of Lockheed's Huntsville Research & Engineering Center. This report is Volume III of a four-part final report, as required to fulfill Contract NAS7-761. This work was sponsored by the Liquid Propulsion Section of Jet Propulsion Laboratories, Mr. Wolfgang Simon, Technical Manager.

This document constitutes Volume III of the four-part final report. The other three volumes, printed separately are:

Volume I - "Summary Volume - Method of Characteristics Nozzle and Plume Programs," LMSC-HREC D162220-I.

Volume II - "User's Manual - Method of Characteristics Plot Program," LMSC-HREC D162220-II.

Volume IV - "User's Manual - Variable O/F Method-of-Characteristics Program for Nozzle and Plume Analyses," LMSC-HREC D162220-IV.

REVISION NOTICE

Lockheed Missiles & Space Company, Huntsville Research & Engineering Center Technical Report HREC 7761-3 (D162220-III), entitled "Solution of Non-Isoenergetic Supersonic Flows by Method of Characteristics," dated July 1971 is revised as indicated below:

Revision A affects title page and pages ii, iii and 68.

SUMMARY

This is one of a series of reports dealing with the calculation of supersonic flow fields by the method of characteristics. This report deals with the theoretical approach to the solution of these flow fields while subsequent reports will compare the theory with experiment and discuss in detail a computer program which was derived to implement the numerical solution of the flow equations. This versatile program has a flexible set of boundary conditions enabling the calculation of nozzles, plumes and many other complex flow fields. A user's guide for this program is contained in Volume IV, "User's Manual - Variable O/F Method-of-Characteristics Program for Nozzle and Plume Analyses," LMSC-HREC D162220-IV.

A complete derivation of the equations of motion for reacting gas systems is presented in this report. This derivation clearly illustrates the underlying assumptions that were made to arrive at the more familiar system of equations which was finally treated. An important consequence of this derivation is that, for the reaction assumptions which were made, the thermochemistry was shown to be uncoupled from the flow solution and as such could be solved separately. In addition the method of characteristics equations are shown to be formally the same for ideal, frozen, and equilibrium reacting gas mixtures.

The two dimensional and axisymmetric characteristic equations are cast in finite difference form. These equations apply only in regions of the flow field where transport properties can be neglected. A shock wave solution is presented, and numerical techniques necessary to effect the calculation are described. The shock wave solution then acts as a patching line between regions in which characteristic relations apply.

A discussion of the mesh construction necessary to apply the local point solutions in the proper fashion is also given.

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SYMBOLS AND NOTATIONS

<u>Symbol</u>	<u>Description</u>
t	time
V	volume
A	area, chemical symbol
ρ	mass density
q	velocity
q'	diffusion velocity
ν	reaction coefficient
m	mass
λ	progress variable
$\bar{\sigma}$	stress tensor
$\bar{\delta}$	unit tensor
$\bar{\tau}$	viscous stress tensor
\bar{f}	body force vector
p	hydrostatic pressure
e	internal energy per unit mass
\bar{Q}	heat flux vector
h	enthalpy per unit mass
s	entropy per unit mass
T	temperature
c	mass fraction

<u>Symbol</u>	<u>Description</u>
μ	Gibbs potential, Mach angle
ΔG	Gibbs free energy change
λ^o	equilibrium progress variable
R_u	universal gas constant
W	molecular weight
γ	isentropic exponent
R	local value R_u/W_m
a^2	speed of sound squared
u, v	velocity components
β	characteristic slope
x, r	position coordinates
θ	inclination of flow vector with respect to x axis
n, t	normal and streamline direction
δ	equation modifier, turning angle
ϵ	shock angle
M	Mach number
E	error function
ϕ	necessary information to describe point
ψ	operation function
j, k	known and partially known characteristic
∇	Nabla
D/Dt	substantial derivative

<u>Superscripts</u>	<u>Description</u>
-	vector, also denotes averaged quantity
=	tensor - dyad
T	transpose
F	forward
R	reverse
(n)	n th iteration

<u>Subscripts</u>	
i	i th species, otherwise where defined
k	k th reaction
l	summation index
m	pertaining to the mixture
e, f	equilibrium and frozen
0	reference condition
N. E.	non-equilibrium

Section 1 INTRODUCTION

The method of characteristics is known to be an accurate means of calculating supersonic flow fields. Since the advent of modern high speed digital computers, this method has recieved much attention because of its accuracy and, in spite of, its complexities. The equations found in this report, although perhaps different in minor ways, are those which have been known and used for half a century. It is felt though that the manner in which these concepts have been combined to result in a useful, flexible tool for rapid calculations is unique.

A complete derivation of the equations of motion for reacting gas mixtures is presented in this report. This was done so that the consequences of assumptions necessary to arrive at the simple forms ultimately treated can be examined. For the special types of reactions treated it is shown that the thermochemistry can be completely separated from the flow solution thus greatly simplifying the entire calculational procedure.

In spite of the almost universal application which the method has recieved, very few descriptions of the mesh construction techniques necessary to apply this method have been documented. It is the intention of this report to present this important portion of the theory. A functional description of the mesh construction will be attempted in the hope that it will enhance the understanding of this facet of the technique.

Section 2

THE FUNDAMENTAL EQUATIONS FOR FLOW OF REACTING GAS MIXTURES

2.1 DERIVATION OF EQUATIONS FOR UNSTEADY NONEQUILIBRIUM FLOW

2.1.1 The Continuity Equation

In a flow system of gaseous mixtures in which chemical reactions take place, the principle of conservation of mass of each chemical species, when applied to a control volume V bounded by a control surface A , may be written as

$$\frac{\partial}{\partial t} \iiint_V \rho_i dV = - \oint_A \rho_i \bar{q}_i \cdot d\bar{A} + \iiint_V \frac{\delta \rho_i}{\delta t} dV \quad (2-1)$$

$$i = 1, 2, \dots, n$$

where ρ_i is the partial density of the i^{th} species; \bar{q}_i the velocity vector of the center of mass of the i^{th} species, $d\bar{A}$ the outward differential area vector on the control surface A ; dV the differential volume element; $\delta \rho_i / \delta t$ the rate of increase of ρ_i due to either internal or external sources such as chemical reaction and mass additions; and n is the total number of chemical species in the mixture.

The above equation simply states that, for the i^{th} species, the mass rate of increase inside the control volume is equal to the net rate of mass flow into the control volume plus the rate of mass produced due to chemical reactions and mass addition. In the following, we shall, however, exclude mass addition from external sources.

The first integral on the right-hand side of Equation (2-1) may be transformed by means of Gauss' theorem

$$\oint_A \bar{Q}(\bar{r}, t) \cdot d\bar{A} = \iiint_V \nabla \cdot \bar{Q}(\bar{r}, t) dV$$

where $\bar{Q}(\bar{r}, t)$ may be any continuous vector field (functions of position vector \bar{r} and time t) defined inside and on the boundary of the control volume V . Also, in the Eulerian coordinate system which we use here, the control volume is not a function of time, and the order of differentiation and integration may be interchanged, i.e.,

$$\frac{\partial}{\partial t} \iiint_V \rho_i dV = \iiint_V \frac{\partial \rho_i}{\partial t} dV$$

Hence, Equation (2-1) becomes

$$\iiint_V \left[\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \bar{q}_i) - \frac{\delta \rho_i}{\delta t} \right] dV = 0 \quad (2-2)$$

Since the volume V under consideration is arbitrary, the only way for Equation (2-2) to be valid for all V is for the integrand to vanish. We therefore have

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i (\bar{q} + \bar{q}'_i)] = \frac{\delta \rho_i}{\delta t} \quad (2-3)$$

$$i = 1, 2, \dots, n$$

where we have replaced \bar{q}_i by $\bar{q} + \bar{q}'_i$. \bar{q} is the velocity of the center of mass of the mixture at (\bar{r}, t) and \bar{q}'_i is the diffusion velocity of the i^{th} species with respect to the mass center of the mixture.

Equation (2-3) is known as the species continuity equation. It is valid for each chemical species at each internal quantum state. We shall, however, assume that the various internal modes of motion are fully excited and are in equilibrium with each other. It is well known that this is approximately the case for the translational and rotational degrees of freedom where the equilibrium value is attained in a few collisions. In general, the vibrational degree of freedom approaches the equilibrium state somewhat more slowly, except at very high temperatures. As chemical reactions usually occur at high temperatures, this approximation is often justified.

If one sums up the n equations represented by Equation (2-3) and utilizes the relationship between the mass density ρ of the mixture and the species density ρ_i

$$\rho = \sum_{i=1}^n \rho_i \quad (2-4)$$

the requirement for the diffusion velocity that

$$\sum_{i=1}^n \rho_i \bar{q}_i' = \sum_{i=1}^n \rho_i (\bar{q}_i - \bar{q}) = \rho \bar{q} - \rho \bar{q} = 0, \quad (2-5)$$

and the conservation of total mass for chemical reactions,

$$\sum_{i=1}^n \frac{\delta \rho_i}{\delta t} = 0 \quad (2-6)$$

one readily obtains

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{q}) = 0 \quad (2-7)$$

Equation (2-7) has the usual form of mass conservation or global continuity equation. It can be written alternatively as

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \bar{q} = 0 \quad (2-7a)$$

by means of Euler's derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{q} \cdot \nabla$$

The species continuity Equation (2-3) may be written in more convenient forms. By making use of the global continuity equation and introducing the mass fraction $c_i (= \rho_i / \rho)$, Equation (2-3) becomes

$$\rho \frac{Dc_i}{Dt} + \nabla \cdot (\rho c_i \bar{q}_i') = \frac{\delta \rho_i}{\delta t} \quad (2-8)$$

The term on the right-hand side of Equation (2-8) may be put into terms of progress variables of the chemical reactions.

Supposing there are r independent reactions occurring in a mixture of n species, then a typical k^{th} reaction may be represented by the general form

$$\sum_{i=1}^n \nu_{ik} A_i = 0, \quad k = 1, 2, \dots, r \quad (2-9)$$

where A_i is the chemical symbol for component i and ν_{ik} is the number of grams of component i produced per gram of reaction k . Since the mass of a reacting system is conserved while the number of moles in such a system is not, it is more convenient to use the gram basis rather than the mole basis in our discussion of chemical reactions. The coefficient ν_{ik} is negative if i is a reactant and positive if i is a product of the reaction k .

If component i does not participate in reactions k , then the corresponding ν_{ik} is zero.

It follows, obviously, from the above description that if there is no mass addition from external sources,

$$\sum_{i=1}^n \nu_{ik} = 0, \quad k = 1, 2, \dots, r \quad (2-10)$$

Furthermore, the changes of mass of the components in the system as a result of the k^{th} reaction are related by

$$\frac{d_k m_1}{\nu_{1k}} = \frac{d_k m_2}{\nu_{2k}} = \dots = \frac{d_k m_n}{\nu_{nk}}, \quad k = 1, 2, \dots, r \quad (2-11)$$

Now we introduce a progress variable λ_k for the k^{th} reaction and define it as the grams of reaction occurred per gram of original reactants. As a result of this definition, we have

$$d\lambda_k = \frac{d_k m_i}{\nu_{ik} m} \quad (2-12)$$

where m is the total mass of the fluid system. We note that because of Equation (2-11), $d\lambda_k$ is independent of species i .

The rate of change of mass of i^{th} species due to all the reactions is therefore,

$$\frac{dm_i}{dt} = m \sum_{k=1}^r \nu_{ik} \frac{d\lambda_k}{dt}, \quad i = 1, 2, \dots, n \quad (2-13)$$

or, in terms of mass density

$$\frac{d\rho_i}{dt} = \rho \sum_{k=1}^r \nu_{ik} \frac{d\lambda_k}{dt} = \frac{\delta\rho_i}{\delta t} \quad (2-13a)$$

With this relationship the species continuity Equation (2-8) becomes

$$\frac{Dc_i}{Dt} + \frac{1}{\rho} \nabla \cdot (\rho c_i \bar{q}_i') = \sum_{k=1}^r \nu_{ik} \frac{D\lambda_k}{Dt} \quad (2-14)$$

It will be shown later that the time rate of change of progress variable $d\lambda_k/dt$ is directly related to the temperature and pressure variations in the flow field.

It is worth noting that all the above equations are extremely general in their validity. That is, they hold true for all flow systems including non-equilibrium chemical reactions and irreversible transport effects such as viscosity, conductivity and diffusivity.

2.1.2 The Momentum Equation

By applying the principle of conservation of momentum to a differential element in the flow field, one can derive, in vector form,

$$\frac{\partial(\rho \bar{q})}{\partial t} + \nabla \cdot (\rho \bar{q} \bar{q}) = \nabla \cdot \bar{\sigma} + \sum_{i=1}^n \rho_i \bar{f}_i \quad (2-15)$$

where $\bar{q} \bar{q}$ is a dyadic product of the velocity vector \bar{q} by itself and \bar{f}_i is the body force exerted on the i^{th} species per unit mass. The stress tensor $\bar{\sigma}$ is sometimes written in the form

$$\bar{\sigma} = -p \bar{\delta} + \bar{\tau} \quad (2-16)$$

Here, p is the hydrostatic pressure usually defined as $-(\sigma_{11} + \sigma_{22} + \sigma_{33})/3$; $\bar{\delta}$ the unit tensor; and $\bar{\tau}$ the viscous part of the stress tensor.

Putting Equation (2-16) into Equation (2-15), we have the well known Navier-Stokes equation for compressible fluid flow,

$$\frac{\partial(\rho \bar{q})}{\partial t} + \nabla \cdot (\rho \bar{q} \bar{q}) = -\nabla p + \nabla \cdot \bar{\tau} + \sum_{i=1}^n \rho_i \bar{f}_i \quad (2-17)$$

In this equation the five terms are, respectively, the non-stationary and convective rate of change of momentum per unit volume, the net hydrostatic pressure force and the viscous stress force acting on the surface of the unit volume, and the body forces per unit volume.

By using the continuity equation (2-7), Equation (2-17) may be written as

$$\frac{D\bar{q}}{Dt} = \frac{\partial \bar{q}}{\partial t} + \bar{q} \cdot \nabla \bar{q} = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \bar{\tau} + \frac{1}{\rho} \sum_{i=1}^n \rho_i \bar{f}_i \quad (2-18)$$

For isotropic, Newtonian fluids, the viscous stress tensor $\bar{\tau}$ in Equations (2-17) and (2-18) can be shown to be related to the velocity gradients (strain rates) by the following formula

$$\bar{\tau} = \psi_1 (\nabla \cdot \bar{q}) \bar{\delta} + \psi_2 (\nabla \bar{q} + (\nabla \bar{q})^T)/2 \quad (2-19)$$

In which $(\nabla \bar{q})^T$ denotes the transpose of the tensor $\nabla \bar{q}$, and ψ_1 and ψ_2 are called the first and second coefficient of viscosity of the fluid, respectively. These coefficients are usually temperature dependent.

When the body forces are negligible, as is usually the case for compressible flow, and if the viscosity effects are small, then we arrive

at the familiar Euler equation of motion

$$\frac{D\bar{q}}{Dt} = \frac{\partial \bar{q}}{\partial t} + \bar{q} \cdot \nabla \bar{q} = -\frac{1}{\rho} \nabla p \quad (2-20)$$

We note at this point that chemical reactions do not alter the forms of global continuity equation or equations of motion.

2.1.3 The Energy Equation

The most general form of energy equation, according to the first law of thermodynamics or the law of conservation of energy, can be written as

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho \left(e + \frac{1}{2} q^2 \right) \right] + \nabla \cdot \left[\rho \bar{q} \left(e + \frac{1}{2} q^2 \right) \right] = & -\nabla \cdot \bar{Q} + \nabla \cdot (\bar{\sigma} \cdot \bar{q}) \\ & + \sum_{i=1}^n \rho_i (\bar{q} + \bar{q}_i') \cdot \bar{f}_i \end{aligned} \quad (2-21)$$

where e is the internal energy per unit mass of the gas mixture; q the magnitude of the velocity; and \bar{Q} the conduction heat flux vector.

Equation (2-21) simply states that, based on unit volume of a fluid element, the total rate of increase of internal and kinetic energy due to local and convective changes (the first two terms) is equal to the heat conducted into the volume (the third term) plus the work done on the fluid element due to stresses (the fourth term) and the work done on the element by the body forces (the last term).

In writing Equation (2-21), all that has been neglected is the energy transferred due to radiation, which if necessary, can be added to the equation as an extra term.

Needless to say, the microscopic quantum effects (interchange of

energy and mass) are not considered in Equation (2-21) as it has been implied by the classical first law of thermodynamics.

Using Equation (2-16) and introducing the enthalpy per unit mass

$$h \equiv e + p/\rho$$

Equation (2-21) can be easily rearranged to give

$$\begin{aligned} \frac{\partial}{\partial t} \rho \left(h + \frac{1}{2} q^2 \right) + \nabla \cdot \left[\rho \bar{q} \left(h + \frac{1}{2} q^2 \right) \right] &= \frac{\partial p}{\partial t} + \nabla \cdot (\bar{\tau} \cdot \bar{q} - \bar{Q}) \\ &+ \sum_{i=1}^n \rho_i (\bar{q} + \bar{q}'_i) \cdot \bar{f}_i \end{aligned} \quad (2-22)$$

Or, if we subtract the continuity Equation (2-7) from Equation (2-22), we obtain

$$\frac{D}{Dt} \left(h + \frac{1}{2} q^2 \right) = \frac{1}{\rho} \frac{\partial p}{\partial t} + \frac{1}{\rho} \nabla \cdot (\bar{\tau} \cdot \bar{q} - \bar{Q}) + \frac{1}{\rho} \sum_{i=1}^n \rho_i (\bar{q} + \bar{q}'_i) \cdot \bar{f}_i \quad (2-23)$$

This is the energy equation in which all the transport properties - viscosity, conductivity and diffusivity, have been taken into consideration.

2.2.4 The Entropy Equation

The general thermodynamics equation with chemical reactions may be written as

$$T ds = dh - \frac{1}{\rho} dp - \sum_{i=1}^n \mu_i dc_i \quad (2-24)$$

where s is the entropy per unit mass of the mixture and μ_i the chemical potential per mole of the chemical species i .

For a flow system, we can write Equation (2-24) in terms of substantial derivatives

$$T \frac{Ds}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} - \sum_{i=1}^n \mu_i \frac{Dc_i}{Dt} \quad (2-25)$$

Now, multiplying the momentum Equation (2-18) by \bar{q} , one gets

$$\bar{q} \cdot \frac{\partial \bar{q}}{\partial t} + \bar{q} \cdot (\bar{q} \cdot \nabla \bar{q}) = - \frac{1}{\rho} \nabla p \cdot \bar{q} + \frac{1}{\rho} (\nabla \cdot \bar{\tau}) \cdot \bar{q} + \frac{1}{\rho} \bar{q} \cdot \sum_{i=1}^n \rho_i \bar{f}_i \quad (2-26)$$

If this equation is subtracted from Equation (2-23) the result is

$$\frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} = \frac{1}{\rho} \bar{\tau} : \nabla \bar{q} - \frac{1}{\rho} \nabla \cdot \bar{Q} + \frac{1}{\rho} \sum_{i=1}^n \rho_i \bar{q}'_i \cdot \bar{f}_i \quad (2-27)$$

where the symbol $:$ is a double dot product of two second order terms. It is defined as

$$\bar{A} : \bar{B} = \sum_{j=1}^3 \sum_{k=1}^3 A_{jk} B_{jk}$$

so,

$$\bar{\tau} : \nabla \bar{q} = \sum_{j=1}^3 \sum_{k=1}^3 \tau_{jk} \frac{\partial q_j}{\partial x_k}$$

Now, substituting Equation (2-27) into Equation (2-25), we readily obtain

$$T \frac{Ds}{Dt} = \frac{1}{\rho} \bar{\tau} : \nabla \bar{q} - \frac{1}{\rho} \nabla \cdot \bar{Q} + \frac{1}{\rho} \sum_{i=1}^n \rho_i \bar{q}'_i \cdot \bar{f}_i - \sum_{i=1}^n \mu_i \frac{Dc_i}{Dt} \quad (2-28)$$

This equation states that the total rate of entropy production, in energy per

unit mass per unit time, is equal to the sum of the individual rate of entropy production due to viscosity (the second term), conductivity (third term), diffusivity (fourth term) and chemical reactions (last term). The fourth terms on the right-hand side of Equation (2-28) are all positive quantities. They are sometimes known as the dissipation terms.

The last term in Equation (2-28) may, with the help of Equation (2-14), be written as

$$- \sum_{i=1}^n \mu_i \frac{Dc_i}{Dt} = - \sum_{i=1}^n \mu_i \left[\sum_{k=1}^r \nu_{ik} \frac{D\lambda_k}{Dt} - \frac{1}{\rho} \nabla \cdot (\rho c_i \bar{q}'_i) \right] \quad (2-29)$$

which, if the diffusion velocity is neglected, becomes

$$- \sum_{i=1}^n \mu_i \frac{Dc_i}{Dt} = - \sum_{k=1}^r \Delta G_k \frac{D\lambda_k}{Dt} \quad (2-30)$$

with

$$\Delta G_k = \sum_{i=1}^n \nu_{ik} \mu_i \quad (2-31)$$

It is to be noted here that the Gibbs free-energy change due to k^{th} reaction, ΔG_k , vanishes for equilibrium chemical reactions.^[1]

2.2 THE EQUATION SYSTEMS FOR STEADY NON-EQUILIBRIUM FLOWS OF REACTING GAS MIXTURES WITHOUT TRANSPORT EFFECTS

For steady, adiabatic, inviscid and non-diffusive flows, the general equations derived in the last section may be reduced to relatively simple forms.

2.2.1 The Continuity Equation

The global continuity equation (2-7) becomes

$$\nabla \cdot (\rho \bar{q}) = 0 \quad (2-32)$$

The species continuity equation (2-14) reduces to

$$\frac{Dc_i}{Dt} = \sum_{k=1}^r \nu_{ik} \frac{D\lambda_k}{Dt}, \quad i = 1, 2, \dots, n \quad (2-33)$$

In the following we shall show that the variation of progress variable λ_k with respect to time is directly related to the temperature and pressure variations.

Following the method of Kirkwood and Crawford [2], we separate λ_k into two parts

$$\lambda_k = \lambda_k^0 + \xi_k \quad (2-34)$$

The parameter λ_k^0 is the equilibrium value of the progress variable for the k^{th} reaction for the instantaneous local temperature, pressure and composition. The variable ξ_k is the measure of the deviation of the chemical reaction from equilibrium; i.e., it is the lag of the k^{th} reaction in its attempt to maintain equilibrium.

The equilibrium value of λ_k^0 is determined by the condition that the Gibbs free-energy change for reaction k vanishes, i.e.,

$$\Delta G_k = 0 \quad \text{at} \quad \lambda_k = \lambda_k^0 \quad (2-35)$$

or, by Equation (2-31)

$$\sum_{k=1}^r \nu_{ik} \frac{D\lambda_k}{Dt} = 0 \quad (2-36)$$

Since

$$d\mu_i = -s_i dT + \frac{1}{\rho_i} dp + \sum_{l=1}^n \left| \frac{\partial \mu_i}{\partial c_l} \right| dc_l \quad (2-37)$$

Equation (2-36) becomes

$$\sum_{i=1}^n \sum_{\ell=1}^n \nu_{ik} \frac{\partial \mu_i}{\partial c_\ell} \frac{Dc_\ell}{Dt} = \Delta s_k \frac{DT}{Dt} - \Delta \left(\frac{1}{\rho} \right)_k \frac{Dp}{Dt} \quad (2-38)$$

where

$$\Delta s_k = \sum_{i=1}^n \nu_{ik} s_i, \quad \Delta \left(\frac{1}{\rho} \right)_k = \sum_{i=1}^n \nu_{ik} \frac{1}{\rho_i}$$

are respectively the change of specific entropy and specific volume due to k^{th} reaction.

Now if we substitute the species continuity Equation (2-33) for $\lambda_j = \lambda_j^0$ into (2-7) we obtain

$$\sum_{i=1}^n \sum_{\ell=1}^n \sum_{j=1}^r \nu_{ik} \nu_{\ell j} \frac{\partial \mu_i}{\partial c_\ell} \frac{D\lambda_j^0}{Dt} = \Delta s_k \frac{DT}{Dt} - \Delta \left(\frac{1}{\rho} \right)_k \frac{Dp}{Dt} \quad (2-39)$$

$$k = 1, 2, \dots, r$$

This equation holds true for flow systems of reacting mixtures under complete chemical equilibrium.

2.2.2 The Momentum Equation

Here, we obtain from Euler's equation of motion (2-20),

$$\bar{q} \cdot \nabla \bar{q} = - \frac{1}{\rho} \nabla p \quad (2-40)$$

2.2.3 The Energy Equation

From Equation (2-23) the steady state energy equation for inviscid,

adiabatic flows with negligible body forces is simply

$$h + \frac{1}{2} q^2 = h_o = \text{const.} \quad (2-41)$$

where h_o is the stagnation enthalpy per unit mass of the mixture. The local specific enthalpy of the mixture is to be evaluated by

$$h = \sum_{i=1}^n h_i c_i \quad (2-41a)$$

in which h_i is the partial specific enthalpy.

2.2.4 The Entropy Equation

From Equation (2-28) and (2-30) we have simply

$$\bar{q} \cdot \nabla s = - \sum_{k=1}^r \Delta G_k \frac{D\lambda_k}{Dt} \quad (2-42)$$

where ΔG_k was given by Equation (2-31).

In the above, we can count a total of $n+r+4$ equations, namely, n equations of (2-33), r equations of (2-39), Equations (2-32), (2-40), (2-41) and (2-42). Yet we have a total number of $n+r+6$ dependent variables, namely, $c_1, c_2, \dots, c_n, \lambda_1, \lambda_2, \dots, \lambda_r, p, T, \rho, h, s$, and \bar{q} . Thus, two more equations are needed. The first one has already been implied by the definition of c_i , i.e., (Equation (2-4)).

$$\sum_{i=1}^n c_i = 1 \quad (2-43)$$

The second one is provided by the equation of state of the gas mixture

$$p = R_u \rho T \sum_{i=1}^n c_i / w_i \quad (2-44)$$

where R_u is the universal gas constant and W_i the molecular weight of the i^{th} species.

This completes the system of the basic governing equations for any reacting flow without transport effects.

When the reactions between components of the gas mixture are known and the boundary conditions adequately specified, one should be able to solve the non-equilibrium flow system.

Section 3

FROZEN AND EQUILIBRIUM FLOWS

3.1 FROZEN FLOW

Under many circumstances, chemical reactions may proceed so slowly that there is hardly any change in composition of the fluid during the time for it to traverse the whole region of flow field of interest. In the limit the mixture may be considered as having fixed composition. Such a flow field is usually described as a "frozen flow." Under a frozen flow condition, the mixture behaves as a single perfect gas. The species continuity equation does not come into picture while the equation of state becomes

$$p = R_u \rho T / W_m$$

where W_m is the fixed molecular weight of the mixture.

Under frozen flow assumptions, the basic governing equations for steady flow of gas mixture without transport effects are as follows:

Continuity:

$$\nabla \cdot (\rho \bar{q}) = 0 \quad (3-1)$$

Momentum:

$$\bar{q} \cdot \nabla \bar{q} = - \frac{1}{\rho} \nabla p \quad (3-2)$$

Energy:

$$h + \frac{1}{2} \bar{q}^2 = h_0 \quad (3-3)$$

Here, h is a function of temperature only.

Entropy:

$$s = \text{constant along a streamline} \quad (3-4)$$

State:

$$p = R_u \rho T / W_m \quad (3-5)$$

The above equations are the usual gas dynamic equations for inviscid, non-conducting, non-diffusive compressible flow without chemical reactions.

It should be stated here that the validity of Equation (3-4) rests upon the assumption of zero transport effects. This means that discontinuities such as shock waves should, strictly speaking, be excluded, since the appearance of shock waves indicates the existence of transport phenomena. However, experience tells us that shock waves usually occur in a very narrow region (in this region viscosity and diffusivity predominate) and we can still apply the isentropic criteria on each side of the shock wave but not across it.

3.2 EQUILIBRIUM FLOW

Equilibrium flows are defined as flows in which the mixture is at chemical equilibrium at all instants and everywhere in the flow field. Physically, this is approximately the case when the chemical reactions in the mixture proceed so fast such that the reactions are "completed" in a time interval much smaller than the time interval we have reason to be interested in. A reaction is said to be "completed" when there is no further appreciable change in the composition of the mixture.

In this case, the set of governing equations may be again simplified to give:

Global Continuity:

$$\nabla \cdot (\rho \bar{q}) = 0 \quad (3-6)$$

Momentum:

$$\bar{q} \cdot \nabla \bar{q} = - \frac{1}{\rho} \nabla p \quad (3-7)$$

Energy:

$$h_e + \frac{1}{2} q^2 = h_o \quad (3-8)$$

where h_e is the local equilibrium value of specific enthalpy.

Entropy:

$$s = \text{constant along streamlines} \quad (3-9)$$

This is a consequence of Equation (2-28) and the remarks following Equation (2-31). We note that the flow is again isentropic in a shock-free field just as in the case of frozen flow.

We note at this point that chemical reactions do not alter the forms of the above equations as compared to frozen flow case.

State

$$p = R_u \rho T / W_{m,e}(\rho, T) \quad (3-10)$$

with

$$W_{m,e}(\rho, T) = \sum_{i=1}^n c_{ie}/W_i \quad (3-10a)$$

Here, it should be pointed out that the mixture of perfect gases does not behave like a perfect gas.

Species Continuity:

$$\frac{Dc_i}{Dt} = \sum_{k=1}^r \nu_{ik} \frac{D\lambda_k^0}{Dt}, \quad i = 1, 2, \dots, n \quad (3-11)$$

$$\sum_{i=1}^n c_i = 1 \quad (3-12)$$

Chemical Kinetics:

$$\sum_{i=1}^n \sum_{l=1}^n \sum_{j=1}^r \nu_{ik} \nu_{lj} \frac{\partial \mu_i}{\partial c_l} \frac{D\lambda_j^0}{Dt} = \Delta s_k \frac{DT}{Dt} - \Delta \left(\frac{1}{\rho} \right)_k \frac{Dp}{Dt} \quad (3-13)$$

$$k = 1, 2, \dots, r$$

Section 4

UNCOUPLING THE FLOW AND THERMODYNAMICS FOR STEADY, FROZEN OR EQUILIBRIUM FLOWS

For steady flow equation (3-13) can be written

$$\sum_{i=1}^n \sum_{l=1}^n \sum_{j=1}^r \nu_{ik} \nu_{lj} \frac{\partial \mu_i}{\partial c_l} \bar{q} \cdot \nabla \lambda_j^0 - \Delta s_k \bar{q} \cdot \nabla T + \Delta \left(\frac{1}{\rho} \right)_k \bar{q} \cdot \nabla p = 0 \quad (4-1)$$

Since all terms except the gradients of λ_j^0 , T , p are scalar quantities we may write

$$\bar{q} \cdot \left\{ \sum_{i=1}^n \sum_{l=1}^n \sum_{j=1}^r \nu_{ik} \nu_{lj} \frac{\partial \mu_i}{\partial c_l} \nabla \lambda_j^0 - \Delta s_k \nabla T + \Delta \left(\frac{1}{\rho} \right)_k \nabla p \right\} = 0$$

Thus the thermochemical behavior does not depend on the magnitude of the velocity, and assuming that it does not depend on the direction, we have

$$\sum_{i=1}^n \sum_{l=1}^n \sum_{j=1}^r \nu_{ik} \nu_{lj} \frac{\partial \mu_i}{\partial c_l} \nabla \lambda_j^0 - \Delta s_k \nabla T + \Delta \left(\frac{1}{\rho} \right)_k \nabla p = 0 \quad (4-2)$$

Examining now the behavior of the thermodynamic system over an infinitesimal step $d\bar{L}$

$$\sum_{i=1}^n \sum_{l=1}^n \sum_{j=1}^r \nu_{ik} \nu_{lj} \frac{\partial \mu_i}{\partial c_l} d\lambda_j^0 - \Delta s_k dT + \Delta \left(\frac{1}{\rho} \right)_k dp = 0 \quad (4-3)$$

Obviously the above equation does not depend on position or velocity and hence is entirely uncoupled from the flow problem. Using the same approach on Equation (3-11) we find;

$$dc_i - \sum_{k=1}^r \nu_{ik} d\lambda_k^0 = 0 \quad (4-4)$$

The thermochemistry equations (3-11) and (3-13) have been completely divorced from the flow problem and describe the behavior of a mixture of perfect gases under infinitesimal changes in pressure and temperature.

It is no longer necessary to use Equations (4-3) and (4-4) in their differential form. Systems of equations describing the behavior of reacting mixtures are well known and many sophisticated computer programs exist to facilitate the solution of these equations. The NASA-Lewis thermochemical program^[3] was chosen for use in this study for a variety of reasons and, due to the fact that special features of this program were utilized in simplifying the subsequent flow field analysis, other thermochemical programs may not be immediately compatible. This need not, however, preclude their use.

Section 5 PROPERTIES OF THE WORKING GAS

Given the initial reactants, combustion pressure, and total energy the thermochemistry program chosen for use in this analysis evaluates, among other things, the following quantities:

$$T, s, W_m, \gamma$$

where γ , the isentropic exponent, is defined by

$$\gamma = \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_s \quad (5-1)$$

At constant entropy, a series of lower pressures are then evaluated. At each step the enthalpy of the mixture is computed in addition to the quantities listed above. From the conservation of energy, the thermochemical analysis is related to the flow systems by calculating the energy change from the original combustion value. In the flow problem the energy difference is the kinetic energy of the gases. A velocity may then be found corresponding to each pressure. In order to describe the effects of shock waves and other irreversible phenomena the chamber pressure is decreased and the process repeated. In this fashion a tabular description of the behavior of the thermochemical system is constructed. Entropy and velocity are chosen to be the independent quantities and specification of these parameters is then sufficient to uniquely describe the gas properties.

Computer economics dictate that the tabular description occupy as little space as possible. Because of this an accurate interpolation scheme is necessary. Before attempting an explanation of the interpolation scheme a definition of local reference conditions is in order. Usually, for an ideal

gas, reference conditions are chosen to be isentropic stagnation conditions. To arrive at local conditions one need only employ well known gas dynamic equations. For a gas whose isentropic exponent and molecular weight is varying, however, the situation is more complicated. A reference condition is defined which is produced by isentropically stagnating an ideal gas whose isentropic exponent and molecular weight are equal to the local mixture value. The reference temperature is

$$T_o = T + \frac{\gamma-1}{2\gamma R} q^2 \quad (5-2)$$

and the reference pressure is

$$p_o = p \left(\frac{T_o}{T} \right)^{\frac{\gamma}{\gamma-1}} \quad (5-3)$$

where

$$R = R_u / W_m$$

To interpolate between two velocity values (1, 2) use

$$R = (1-h_v) R_1 + h_v R_2 \quad (5-4)$$

$$\gamma = (1-h_v) \gamma_1 + h_v \gamma_2 \quad (5-5)$$

$$T = T_1 + \frac{q_1^2}{2\xi_T R_1} - \frac{q^2}{2\xi_T R} \quad (5-6)$$

$$p = p_1 \left(\frac{T}{T_1} \right)^{\xi p} \quad (5-7)$$

where

$$h_v = \frac{q - q_1}{q_2 - q_1}$$

$$\xi_T = \left(\frac{q_2^2}{2R_2} - \frac{q_1^2}{2R_1} \right) / (T_1 - T_2)$$

$$\xi_p = \ln(p_1/p_2) / \ln(T_1/T_2)$$

and to interpolate between two entropy values use

$$R = (1-hs) R_1 + hs R_2 \quad (5-8)$$

$$\gamma = (1-hs) \gamma_1 + hs \gamma_2 \quad (5-9)$$

$$p = p_1 \exp \left\{ hs' \ln \frac{R_2}{R_1} \right\} \quad (5-10)$$

$$T = (1-hs) T_1 + hs T_2 \quad (5-11)$$

where

$$hs = \frac{s-s_1}{s_2-s_1}$$

$$hs' = \frac{s/R - s_1/R_1}{s_2/R_2 - s_1/R_1}$$

In the following development of the flow equations no further mention is made of the nature of the thermochemistry of the gas. A tabular description of the properties is assumed to exist so that it is immaterial whether the gas is ideal, frozen, or in chemical equilibrium.

Section 6 THE METHOD OF CHARACTERISTICS SOLUTION

6.1 DEVELOPMENT OF THE CHARACTERISTIC EQUATIONS

The continuity equation or conservation of mass is, in vector form,

$$\nabla \cdot (\rho \bar{q}) = 0 \quad (6-1)$$

while the conservation of momentum is

$$-\frac{1}{\rho} \nabla p = \nabla \bar{q}^2 / 2 - \bar{q} \times (\nabla \times \bar{q}) \quad (6-2)$$

The thermodynamic relation is

$$T ds = dh - \frac{dp}{\rho}$$

which can be shown to be

$$T \nabla s = \nabla h - \frac{1}{\rho} \nabla p \quad (6-3)$$

Now

$p = p(\rho, s)$ so that

$$\nabla p = \left(\frac{\partial p}{\partial \rho} \right)_s \nabla \rho + \left(\frac{\partial p}{\partial s} \right)_\rho \nabla s \quad (6-4)$$

The conservation of energy and momentum, and the thermodynamic relation combine to give

$$T \nabla s = -\bar{q} \times (\nabla \times \bar{q}) \quad (6-5)$$

Expansion of (6-1) yields

$$\nabla \cdot (\rho \bar{q}) = \rho \nabla \cdot \bar{q} + \bar{q} \cdot \nabla \rho = 0 \quad (6-6)$$

which when combined with Equation (6-4) gives

$$\left(\frac{\partial p}{\partial \rho} \right)_s \rho \nabla \cdot \bar{q} + \bar{q} \cdot \left(\nabla p - \left(\frac{\partial p}{\partial s} \right)_\rho \nabla s \right) = 0$$

But since $\bar{q} \cdot \nabla s = 0$ and $\left(\frac{\partial p}{\partial \rho} \right)_s^{\frac{1}{2}}$ is defined to be the speed of sound we have

$$\nabla \cdot \bar{q} - \frac{\bar{q}}{a^2} \cdot \nabla a^2 = 0 \quad (6-7)$$

Recalling the definition equation (5-1)

$$\gamma = \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_s = \frac{\rho}{p} \left(\frac{\partial p}{\partial \rho} \right)_s = \frac{\rho}{p} a^2$$

so that

$$a^2 = \gamma R T \quad (6-8)$$

Choosing now a cylindrical coordinate system (Figure 1), in which the flow angle θ is defined to be the angle between the velocity vector and the x axis and where r is the distance from that axis, and in this system expanding Equation (6-7), we have for axisymmetric or two dimensional flow,^[4]

$$\left(1 - \frac{u^2}{a^2} \right) \frac{\partial u}{\partial x} + \left(1 - \frac{v^2}{a^2} \right) \frac{\partial v}{\partial r} + \frac{\sigma v}{r} - \frac{uv}{a^2} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial r} \right) = 0 \quad (6-9)$$

where σ is 0, 1 for two dimensional or axisymmetric flow respectively. Consider a line in the r, x plane inclined to the x axis by the angle $\tan^{-1} \beta$, then the expression for this line (normally called a characteristic line) is

$$\frac{dr}{dx} = \beta$$

But along this line

$$du = \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial r} dr = \left(\frac{\partial u}{\partial x} + \beta \frac{\partial u}{\partial r} \right) dx$$

and

$$dv = \left(\frac{\partial v}{\partial x} + \beta \frac{\partial v}{\partial r} \right) dx$$

then

$$\frac{\partial u}{\partial x} = \frac{du}{dx} - \beta \frac{\partial u}{\partial r} \quad (6-10)$$

and

$$\frac{\partial v}{\partial r} = \frac{1}{\beta} \left(\frac{dv}{dx} - \frac{\partial v}{\partial x} \right) \quad (6-11)$$

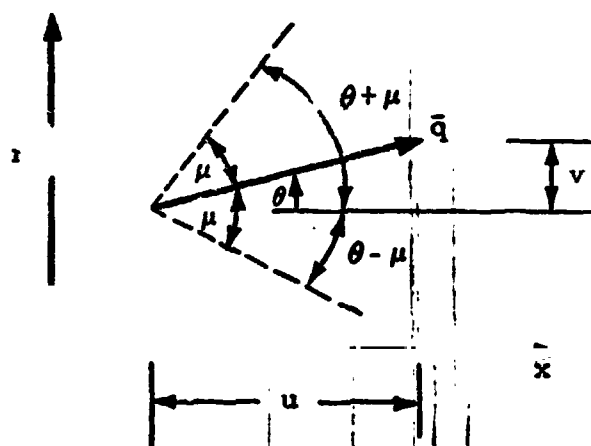


Figure 1

Substitution of Equations (6-10) and (6-11) into Equation (6-9) yields after simplification,

$$\begin{aligned} \left(1 - \frac{u^2}{a^2}\right) \frac{du}{dx} + \frac{1}{\beta} \left(1 - \frac{v^2}{a^2}\right) \frac{dv}{dx} + \frac{\sigma v}{r} - \left\{ \frac{uv}{a^2} + \beta \left(1 - \frac{u^2}{a^2}\right) \right\} \frac{\partial v}{\partial r} \\ - \left\{ \frac{uv}{a^2} + \frac{1}{\beta} \left(1 - \frac{v^2}{a^2}\right) \right\} \frac{\partial v}{\partial x} = 0 \end{aligned} \quad (6-12)$$

Recalling Equation (6-5) and rearranging yields

$$\frac{a^2}{\gamma R} \nabla s = \bar{q} \times (\nabla \times \bar{q})$$

where, for two dimensional or axisymmetric flow,

$$\nabla \times \bar{q} = \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right) \frac{\nabla \times \bar{q}}{|\nabla \times \bar{q}|}$$

and

$$\frac{a^2}{\gamma R} \frac{\partial s}{\partial r} = u \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right)$$

but

$$\frac{\partial s}{\partial n} = \frac{\partial s}{\partial x} \frac{\partial x}{\partial n} + \frac{\partial s}{\partial r} \frac{\partial r}{\partial n}$$

where n is normal to the streamline and

$$\frac{\partial x}{\partial n} = \frac{-y}{r}$$

and

$$\frac{\partial r}{\partial n} = \frac{u}{q}$$

so that

$$\frac{\partial v}{\partial x} = \frac{\partial u}{\partial r} + \frac{a^2}{\gamma R q} \frac{\partial s}{\partial n}$$

Substituting of the above result into Equation (6-12) yields

$$\left(1 - \frac{u^2}{a^2}\right) \frac{du}{dx} + \frac{1}{\beta} \left(1 - \frac{v^2}{a^2}\right) \frac{dv}{dx} + \frac{\sigma v}{r} - \left[\frac{uv}{a^2} + \frac{1}{\beta} \left(1 - \frac{v^2}{a^2}\right)\right] \frac{a^2}{\gamma R q} \frac{\partial s}{\partial n} \quad (6-13)$$

$$- \left\{ \frac{2uv}{a^2} + \beta \left(1 - \frac{u^2}{a^2}\right) + \frac{1}{\beta} \left(1 - \frac{v^2}{a^2}\right) \right\} \frac{\partial u}{\partial r} = 0$$

It is desirable to determine whether there exists some β for which the coefficient of $\frac{\partial u}{\partial r}$ is zero.

$$\beta^2 \left(1 - \frac{u^2}{a^2}\right) + \frac{2uv}{a^2} \beta + \left(1 - \frac{v^2}{a^2}\right) = 0$$

Solving for β yields

$$\beta = \frac{-\frac{uv}{a^2} \pm \left(\frac{u^2}{a^2} - 1\right)^{\frac{1}{2}}}{\left(1 - \frac{u^2}{a^2}\right)}$$

Let

$$\begin{aligned}u &= q \cos \theta \\v &= q \sin \theta \\\mu &= \sin^{-1}(a/q)\end{aligned}$$

Then, after much manipulation,

$$\beta = \tan(\theta + \mu) \quad (6-14)$$

Combination of (6-13) with (6-14) yields then

$$\left(1 - \frac{u^2}{a^2}\right) \frac{du}{dx} + \cot(\theta + \mu) \left(1 - \frac{v^2}{a^2}\right) \frac{dv}{dx} + \frac{\sigma v}{r} - \left\{ \frac{uv}{a^2} + \cot(\theta + \mu) \left(1 - \frac{v^2}{a^2}\right) \right\} \frac{a^2}{\gamma R q} \frac{\partial s}{\partial n} = 0$$

Now

$$ds = \frac{\partial s}{\partial n} dn + \frac{\partial s}{\partial t} dt = \frac{\partial s}{\partial n} dn = \frac{\partial s}{\partial n} \sin \mu dl$$

where t is taken along the streamline and dl is measured along the characteristic line. But

$$dl = \left(1 + \left(\frac{dr}{dx}\right)^2\right)^{\frac{1}{2}} dx = \sec(\theta + \mu) dx$$

Then finally after much algebra

$$d\theta + \frac{\cot \mu}{q} dq + \frac{\sin \mu \cos \mu}{\gamma R} ds + \frac{\sin \mu \sin \theta}{\sin(\theta + \mu)} \frac{\sigma}{r} dr = 0 \quad (6-15)$$

Equation (6-15) is known as the compatibility equation and describes the variation in flow properties along

$$\frac{dr}{dx} = \tan(\theta + \mu) \quad (6-16)$$

These lines are the so-called physical characteristic lines. Locally they are tangent to the Mach lines. Equations (6-15) are often called the hodograph characteristics for two dimensional flow. In axisymmetric flow the existence of the physical dimension causes a coupling of the characteristics so that Equation (6-15) cannot truly be referred to as hodograph characteristics.

It is interesting to note that the only reference to gas properties in the derivation was the use of the definition given in Equation (5-1).

Examination of the four equations (6-15) and (6-16) reveals that there are five unknowns. An additional relation is provided by assuming a linear variation in entropy between the known data points.

6.2 FINITE DIFFERENCE SOLUTION OF THE CHARACTERISTIC EQUATIONS

In order to solve the differential equations (6-15) and (6-16) it is first necessary to write the equations in finite difference form. At times in the flow field certain conditions are known which allow some of the equations to be discarded. These are, of course, the boundary conditions.

$$\frac{\Delta r}{\Delta x}_{1,2} = \tan \bar{\beta}_{1,2} \quad (6-17)$$

$$\Delta \theta_{1,2} \pm \frac{\cot \bar{\mu}_{1,2} \Delta q_{1,2}}{\bar{q}_{1,2}} \pm \frac{\sin \bar{\mu}_{1,2} \cos \bar{\mu}_{1,2} \Delta s_{1,2}}{\bar{r}_{1,2} \bar{R}_{1,2}} + \frac{\sin \bar{\mu}_{1,2} \sin \bar{\theta}_{1,2}}{\sin(\bar{\theta}_{1,2} \mp \bar{\mu}_{1,2})} \frac{\sigma}{\bar{r}_{1,2}} \Delta r_{1,2} = 0 \quad (6-18)$$

where the barred values are averages over the step length and where

$$\bar{\beta}_{1,2} = \bar{\theta}_{1,2} + \delta_{1,2} \bar{\mu}_{1,2}$$

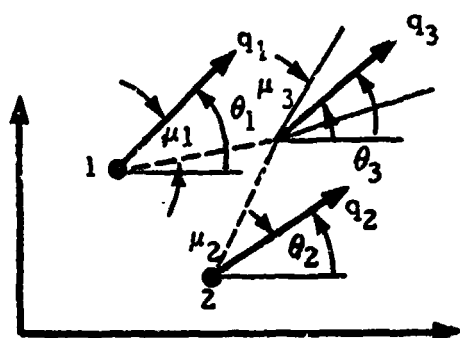
and δ takes on the values

$$\delta_1 = \begin{cases} 1 & \text{for interior solution} \\ 1 & \text{for lower boundary solution} \\ 0 & \text{for upper boundary solution} \end{cases}$$

while

$$\delta_2 = \begin{cases} 1 & \text{for interior solution} \\ 0 & \text{for lower boundary solution} \\ 1 & \text{for upper boundary solution} \end{cases}$$

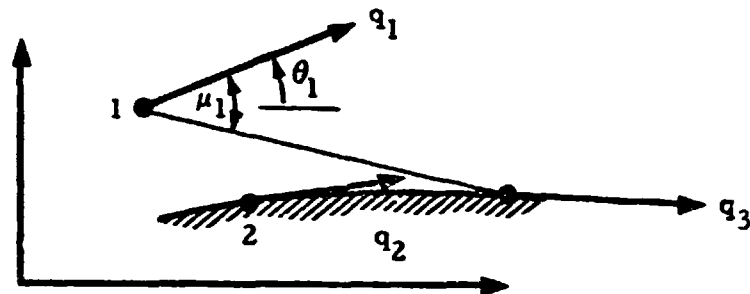
which correspond to the Figures (2a) - (2c) given below



Interior Point

$$\begin{aligned} \delta_1 &= 1 \\ \delta_2 &= 1 \end{aligned}$$

Figure (2a)

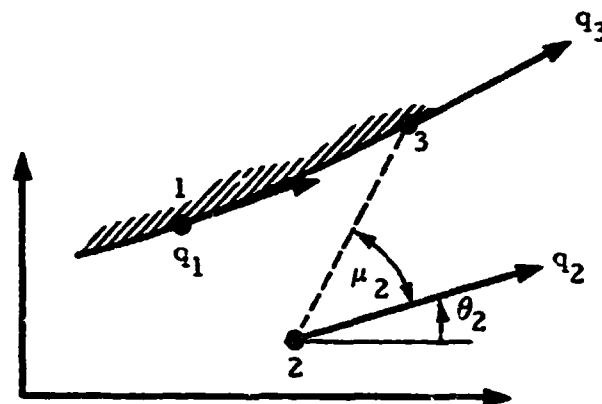


Lower Boundary

$$\delta_1 = 1$$

$$\delta_2 = 0$$

Figure (2b)



Upper Boundary

$$\delta_1 = 0$$

$$\delta_2 = 1$$

Figure (3c)

Notice that for the boundary condition solutions the Equations (6-17) become the streamline equation when δ is zero. For a solid wall solution the flow angle is known while for a pressure boundary the pressure is known.

Five basic cases will be discussed. These are:

- a. interior point solution
- b. upper wall
- c. upper free boundary
- d. lower wall
- e. lower free boundary

The compatability equations are:

a. interior point

$$q_3 = \frac{\theta_1 - \theta_2 + Q_1 q_1 + Q_2 q_2 + G_1 + G_2 - B_1 - B_2}{Q_1 + Q_2} \quad (6-19)$$

$$\theta_3 = \theta_2 + Q_2 (q_3 - q_2) - G_2 + B_2 \quad (6-20)$$

b. upper wall

$$q_3 = \frac{\theta_3 - \theta_2 + G_2 - B_2 + Q_2 q_2}{Q_2} \quad (6-21)$$

where θ_3 is given by the wall equation

c. upper free boundary

$$\theta_3 = \theta_2 + Q_2 (q_3 - q_2) - G_2 + B_2 \quad (6-22)$$

and q_3 is found from the local pressure

d. lower wall solution

$$q_3 = \frac{\theta_1 - \theta_3 + G_1 - B_1 + Q_1 q_1}{Q_1} \quad (6-23)$$

where θ_3 is given by the wall equation

e. lower pressure boundary

$$\theta_3 = \theta_1 - Q_1 (q_3 - q_1) + G_1 - B_1 \quad (6-24)$$

and q_3 is given by the local pressure

where

$$\begin{aligned} Q_{1,2} &= \frac{\cot \bar{\mu}_{1,2}}{\bar{q}_{1,2}} \\ G_{1,2} &= \frac{\sigma \sin \bar{\theta}_{1,2}}{\bar{r}_{1,2}} F_{1,2} \\ B_{1,2} &= \frac{\sin \bar{\mu}_{1,2} \cos \bar{\mu}_{1,2} (s_3 - s_{1,2})}{\bar{R}_{1,2} \bar{Y}_{1,2}} \end{aligned} \quad (6-25)$$

and s_3 is given by

a. interior point

$$s_3 = s_1 + \frac{F_1(s_2 - s_1)}{F_1 + F_2} \quad (6-26)$$

b. and c. upper boundary

$$s_3 = s_1 \quad (6-27)$$

d. and e. lower boundary

$$s_3 = s_2 \quad (6-28)$$

while

$$F_{1,2} = \frac{\sin \bar{\mu}_{1,2} (x_3 - x_{1,2})}{\cos \bar{\beta}_{1,2}} \quad (6-29)$$

An iterative solution is employed to determine the properties at the new point. For the first pass of this solution the barred values are approximated by the conditions at the two known points, e.g.,

$$\bar{\theta}_1 = \theta_1$$

for the first iteration. After the appropriate set of equations has been solved a new estimate of the barred values is made. For example,

$$\bar{\theta}_1 = \frac{\theta_1 + \theta_3}{2}$$

The iterative process is continued until the desired convergence is reached.

Section 7 THE OBLIQUE SHOCK SOLUTION

7.1 DEVELOPMENT OF OBLIQUE SHOCK RELATIONS

Figure 3 illustrates a stream tube passing through an oblique shock wave. This wave, which is extremely thin, will cause an almost instantaneous rise in pressure and temperature. For some distance downstream of the shock wave (in a reacting gas) a non-equilibrium zone will exist followed by a return to chemical equilibrium. The following analysis discusses the fluid flow properties in such a way that the non-equilibrium process need not be specified in order to arrive at an exact solution for the gas properties.

Consider a control surface as shown in the figure. The conservation of mass yields;

$$\rho_2 q_2 A_2 - \rho_1 q_1 A_1 = 0 \quad (7-1)$$

Conservation of momentum gives

$$\begin{aligned} & -(p_1 + \rho_1 q_1^2) A_1 \bar{i}\theta + \frac{p_1 A_1}{\tan \epsilon} \bar{i}n + (p_2 + \rho_2 q_2^2) A_2 \bar{i}\theta' - \frac{p_2 A_2 \bar{i}n'}{\tan(\epsilon - \delta)} \\ & + \int_{A_{N.E.}} p_{N.E.} d\bar{A} - \int_{A_{N.E.}} p_{N.E.} d\bar{A} = 0 \end{aligned}$$

Since each streamline locally undergoes the same process the last two terms of the above equation are equal and opposite. Therefore

$$-(p_1 + \rho_1 q_1^2) A_1 \bar{i}\theta + \frac{p_1 A_1}{\tan \epsilon} \bar{i}n + (p_2 + \rho_2 q_2^2) A_2 \bar{i}\theta' - \frac{p_2 A_2 \bar{i}n'}{\tan(\epsilon - \delta)} = 0 \quad (7-2)$$

Transforming to the ns, ts coordinate system

$$\bar{i}\theta = \sin\epsilon \bar{ns} + \cos\epsilon \bar{ts}$$

$$\bar{in} = -\cos\epsilon \bar{ns} + \sin\epsilon \bar{ts} \quad (7-3)$$

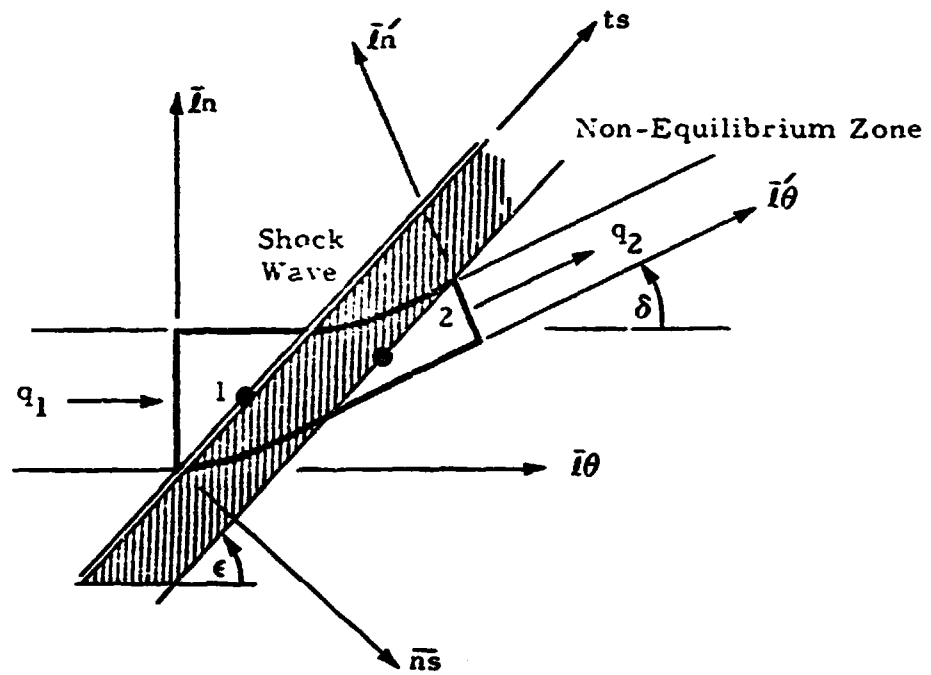


Figure 3

and ..

$$\bar{i}\theta' = \sin(\epsilon-\delta) \bar{ns} + \cos(\epsilon-\delta) \bar{ts}$$

$$\bar{in}' = -\cos(\epsilon-\delta) \bar{ns} + \sin(\epsilon-\delta) \bar{ts} \quad (7-4)$$

So that, after substitution of (7-3) and (7-4) and setting each component to zero, Equation (7-2) becomes,

$$\rho_2 q_2^2 \cos(\epsilon - \delta) A_2 - \rho_1 q_1^2 A_1 \cos \epsilon = 0 \quad (7-5)$$

$$\left(p_1 + \rho_1 q_1^2 \right) A_1 \sin \epsilon + \frac{p_1 A_1}{\tan \epsilon} \cos \epsilon - \left(p_2 + \rho_2 q_2^2 \right) A_2 \sin(\epsilon - \delta)$$

$$- \frac{p_2 A_2 \cos(\epsilon - \delta)}{\tan(\epsilon - \delta)} = 0 \quad (7-6)$$

But from geometry it can be seen that

$$\frac{A_2}{A_1} = \frac{\sin(\epsilon - \delta)}{\sin \epsilon} \quad (7-7)$$

After substitution of Equation (7-7); (7-1), (7-5) and (7-6) become

$$\rho_2 q_2 \sin(\epsilon - \delta) - \rho_1 q_1 \sin \epsilon = 0 \quad (7-8)$$

$$\rho_2 q_2^2 \sin(\epsilon - \delta) \cos(\epsilon - \delta) - \rho_1 q_1^2 \sin \epsilon \cos \epsilon = 0 \quad (7-9)$$

$$p_2 + \rho_2 q_2^2 \sin^2(\epsilon - \delta) - p_1 - \rho_1 q_1^2 \sin^2 \epsilon = 0 \quad (7-10)$$

The above set of relations contains $\epsilon, \delta, p_2, \rho_2, q_2$ as unknown quantities, but

$$p_2 = p(s_2, q_2) ; \rho_2 = \rho(s_2, q_2) \quad (7-11)$$

So that if one variable, say ϵ , is taken as an independent parameter the remaining unknowns (δ, q_2, s_2) may be found by an iterative solution. These equations are, of course, formally the same as the ideal gas solution. The difference lies only in the variation of pressure etc., with entropy and velocity.

It is impossible to determine the location of the new equilibrium shock point location without a detailed description of the non-equilibrium reaction process. It will be assumed therefore that this zone is thin and that no significant errors are introduced by letting the downstream physical location lie on the upstream location.

It has been pointed out previously that the characteristic equation derivation was based on neglecting transport properties and as such is necessarily restricted to continuous regions only. The oblique shock wave relations derived here then are patching lines between the continuous regions.

7.2 ITERATIVE SOLUTION OF THE OBLIQUE SHOCK RELATIONS

Rearranging Equation (7-8) yields;

$$\sin(\epsilon - \delta) = \frac{\rho_1 q_1 \sin \epsilon}{\rho_2 q_2}$$

while squaring both sides of Equation (7-9) and substituting the above relations yields, after simplification;

$$q_2 - q_1 \left\{ \left(\frac{\rho_1}{\rho_2} \right)^2 \sin^2 \epsilon + \cos^2 \epsilon \right\}^{\frac{1}{2}} = 0 \quad (7-12)$$

and Equation (7-10) becomes

$$p_2 + \rho_1 q_1^2 \sin^2 \epsilon \left\{ \frac{\rho_1}{\rho_2} - 1 \right\} - p_1 = 0 \quad (7-13)$$

In functional form Equations (7-12) and (7-13) are just

$$\begin{aligned} G_1(s_2, q_2) &= 0 \\ G_2(s_2, q_2) &= 0 \end{aligned} \quad (7-14)$$

From calculus

$$\begin{aligned} dG_1 &= \frac{\partial G_1}{\partial q_2} dq_2 + \frac{\partial G_1}{\partial s_2} ds_2 \\ dG_2 &= \frac{\partial G_2}{\partial q_2} dq_2 + \frac{\partial G_2}{\partial s_2} ds_2 \end{aligned} \quad (7-15)$$

Now

$$\frac{\partial G_1}{\partial q_2} = 1 + q_1 \left(\frac{q_1}{q_2} \right) \left(\frac{\rho_1}{\rho_2} \right)^2 \sin^2 \epsilon \frac{\partial}{\partial q_2} (\ln \rho_2)$$

$$\frac{\partial G_1}{\partial s_2} = q_1 \left(\frac{q_1}{q_2} \right) \left(\frac{\rho_1}{\rho_2} \right)^2 \sin^2 \epsilon \frac{\partial}{\partial s_2} (\ln \rho_2)$$

$$\frac{\partial G_2}{\partial q_2} = p_2 \frac{\partial}{\partial q_2} (\ln p_2) - \left(\frac{\rho_1}{\rho_2} \right)^2 q_1^2 \sin^2 \epsilon \rho_2 \frac{\partial}{\partial q_2} (\ln \rho_2) \quad (7-16)$$

$$\frac{\partial G_2}{\partial s_2} = p_2 \frac{\partial}{\partial s_2} (\ln p_2) - \left(\frac{\rho_1}{\rho_2} \right)^2 \sin^2 \epsilon \rho_2 \frac{\partial}{\partial s_2} (\ln \rho_2)$$

Rather than calculate the partial derivatives numerically by perturbing the functions $\ln p_2$, $\ln \rho_2$ approximate values for these derivatives will be found by assuming that locally the gas behaves ideally, that is to say

$$\frac{\partial R_2}{\partial s_2} = \frac{\partial R_2}{\partial q_2} = \frac{\partial T o_2}{\partial s_2} = \frac{\partial T o_2}{\partial q_2} = \frac{\partial p o_2}{\partial s_2} = \frac{\partial p o_2}{\partial q_2} = \frac{\partial \gamma_2}{\partial s_2} = \frac{\partial \gamma_2}{\partial q_2} = 0$$

so that

$$\frac{\partial(\ln p_2)}{\partial s_2} \approx \frac{\partial(\ln \rho_2)}{\partial s_2} \approx -\frac{1}{R_2} \quad (7-17)$$

and

$$\frac{\partial(\ln p_2)}{\partial q_2} \approx \gamma_2 \frac{\partial}{\partial q_2} (\ln \rho_2) \approx -\frac{q_2 \rho_2}{p_2} \quad (7-18)$$

writing (7-15) in finite difference form:

$$G_1^{(n+1)} - G_1^{(n)} = \frac{\partial G_1^{(n)}}{\partial q_2} (q_2^{(n+1)} - q_2^{(n)}) + \frac{\partial G_1^{(n)}}{\partial s_2} (s_2^{(n+1)} - s_2^{(n)})$$

$$G_2^{(n+1)} - G_2^{(n)} = \frac{\partial G_2^{(n)}}{\partial q_2} (q_2^{(n+1)} - q_2^{(n)}) + \frac{\partial G_2^{(n)}}{\partial s_2} (s_2^{(n+1)} - s_2^{(n)})$$

Since the root $G_1 = G_2 = 0$ is desired, $G_1^{(n+1)}$, $G_2^{(n+1)}$ are set to zero, resulting in

$$s^{(n+1)} = s^{(n)} + \left(G_2^{(n)} \frac{\partial G_1^{(n)}}{\partial q_2} - G_1^{(n)} \frac{\partial G_2^{(n)}}{\partial q_2} \right) /$$

$$\left(\frac{\partial G_1^{(n)}}{\partial s_2} \frac{\partial G_2^{(n)}}{\partial q_2} - \frac{\partial G_2^{(n)}}{\partial s_2} \frac{\partial G_1^{(n)}}{\partial q_2} \right) \quad (7-19)$$

and

$$q^{(n+1)} = q^{(n)} - \left\{ G_1^{(n)} + \frac{\partial G_1^{(n)}}{\partial s_2} \left(s^{(n+1)} - s^{(n)} \right) \right\} \left/ \frac{\partial G_1^{(n)}}{\partial q_2} \right. \quad (7-20)$$

The iterative solution using Equations (7-19) and (7-20) is continued until the desired convergence of G_1 and G_2 is reached. The solution is completed by

$$\delta = \epsilon - \sin^{-1} \left\{ \frac{\rho_1 q_1}{\rho_2 q_2} \sin \epsilon \right\} \quad (7-21)$$

The first guess to start the solution is an ideal gas solution to the set of equations. If it is indeed an ideal gas under analysis the first guess is exact. These relations are

$$\delta = \epsilon - \tan^{-1} \left\{ \tan \epsilon \left(\frac{1}{M_1^2 \sin^2 \epsilon} + \frac{\gamma_1 - 1}{2} \right) \frac{2}{\gamma_1 + 1} \right\}$$

$$q_2 = q_1 \frac{\cos \epsilon}{\cos(\epsilon - \delta)} \quad (7-22)$$

$$s_2 = s_1 + \frac{R_1}{\gamma_1 - 1} \left\{ \ln \left[\frac{2\gamma_1 M_1^2 \sin^2 \epsilon - (\gamma_1 - 1)}{\gamma_1 + 1} \right] + \gamma_1 \ln \left[\frac{\tan(\epsilon - \delta)}{\tan \epsilon} \right] \right\}$$

Section 8

EXPANSION CORNER - PRANDTL-MEYER FAN

In some cases the flow may be required to negotiate a sharp expansion turn. The problem becomes two dimensional at a sharp corner (it is impossible to conceive of an expansion corner on an axis of symmetry) and may be treated with a Prandtl-Meyer expansion.

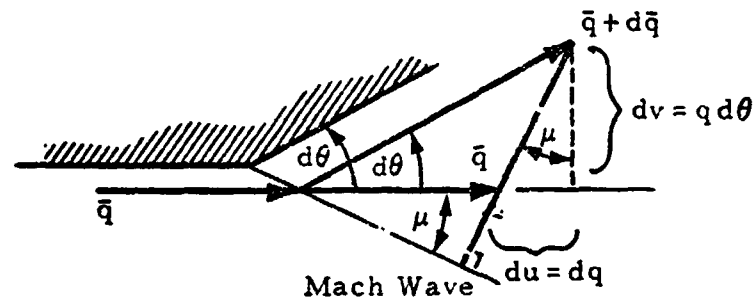


Figure 4

Since a Mach wave will support pressure changes only in a direction normal to itself,^[5]

$$dv = q d\theta$$

$$du = dq$$

$$\frac{du}{dr} = \tan \mu = \frac{1}{\sqrt{M^2 - 1}}$$

or

$$d\theta = \sqrt{M^2 - 1} \frac{dq}{q} \quad (8-1)$$

The solution to Equation (8-1) is a straightforward numerical integration for the case of a known final velocity (free-boundary case). If the turning angle is known, however, and the final velocity is not known, an iterative solution is necessary to determine the upper limit.

$$\int_{q_1}^{q_2} \sqrt{M^2 - 1} \frac{dq}{q} - \Delta\theta = f(q_2) = 0 \quad (8-2)$$

In the mesh construction to be discussed later a fan of rays must be generated to allow a numerical description through a large turning angle. The turning angle is subdivided into a number of small turns, each of which is integrated numerically. Corresponding to each small turn is a Mach wave or characteristic line emanating from the corner.

Section 9
SHOCK NEIGHBORHOOD SOLUTION

Due to the fact that the shock calculation will be employed under several different flow conditions a general setup and notation is used. There are six basic types of calculations as shown in Figures (5a - 5f).

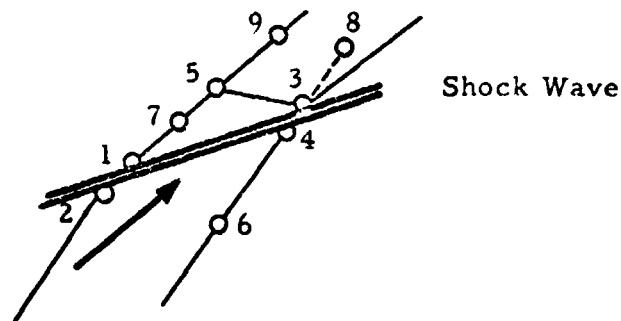


Figure 5a - Interior Right-Running Shock Wave

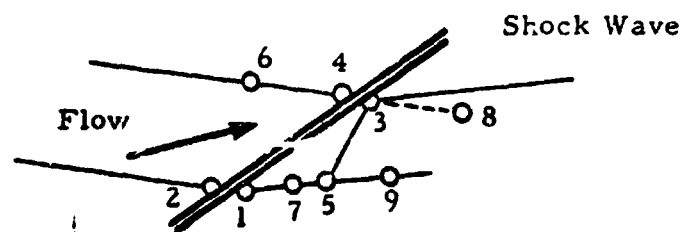


Figure 5b - Interior Left-Running Shock Wave

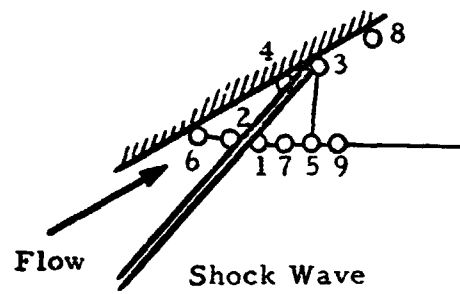


Figure 5c - Solid or Free Upper Wall Interacting with Left-Running Shock

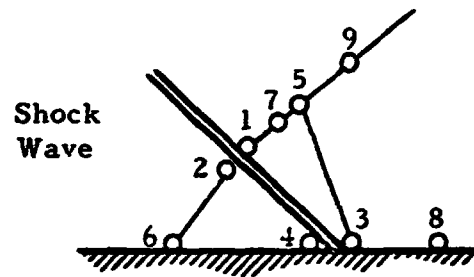


Figure 5d - Solid or Free Lower Wall Interacting with Incident Right-Running Shock Wave

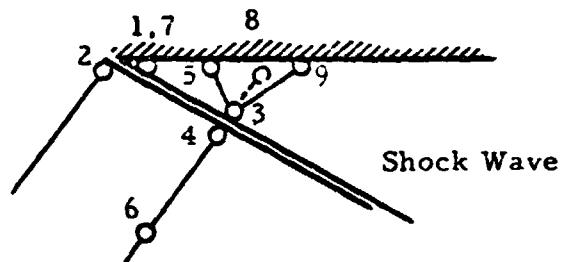


Figure 5e - Solid or Free Upper Wall Interacting with Reflected Shock Wave or Attached Shock Wave with Insufficient Downstream Information

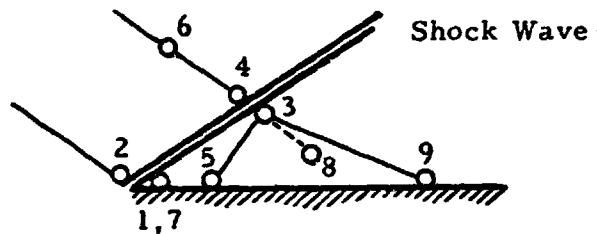


Figure 5f - Solid or Free Lower Wall Interacting with Reflected Shock Wave or Attached Shock Wave with Insufficient Downstream Information

Let

$$\delta_i = 1, -1, -1, 1, 1, -1$$

$$\delta_b = 1, 1, 0, 0, 1, 1$$

$$\delta_w = 1, 1, 1, 1, 0, 0$$

for the six cases, respectively.

The angle that line 6-8 makes with the axis is

$$\alpha_4 = \left\{ \theta_8 + \theta_6 + \delta_i \delta_b (\mu_8 + \mu_6) \right\} / 2$$

while the angle that line 7, 9 makes with the axis is

$$\alpha_5 = \left\{ \theta_9 + \theta_7 + \delta_i \delta_w (\mu_9 + \mu_7) \right\} / 2$$

while the angle of the shock wave is

$$\alpha^{(n)} = \left\{ \theta_2 + \epsilon_2 + (\theta_4 + \epsilon_4)^{(n)} \right\} / 2 \quad (9-1)$$

For an initial approximation let $(\theta_4 + \epsilon_4)^{(0)} = \theta_2 + \epsilon_2$ and compute the physical location of r_4, x_4 which is just the intersection of the shock wave and the line 6-8.

A linear interpolation between the flow values at points 6 and 8 is used to determine the local flow properties at point 4. A shock angle is then determined.

$$\epsilon_4^{(n)} = (\theta + \epsilon)_4^{(n)} - \theta_4^{(n)}$$

The oblique shock solution of section c is used to determine the flow properties at 3 across the shock wave.

It is now necessary to make a characteristic calculation to determine whether the new shock solution is the correct one. In order to do this a physical characteristic line is drawn from point 3 and the intersection of this line and line 7-9 is point 5. In the cases shown in Figure 5e and 5f point 9 is not known. An estimate compatible with the shock slope is made using a characteristic solution.

For a first approximation to the slope of the line let

$$\theta_5^{(n,o)} = \theta_3^{(n)} \quad \text{and let} \quad \mu_5^{(n,o)} = \mu_3^{(n)}$$

then the characteristic line makes the angle

$$\alpha_3^{(n,m)} = \left\{ \theta_5^{(n,m)} + \theta_3^{(n)} - \delta_i \left(\mu_5^{(n,m)} + \mu_3^{(n)} \right) \right\} / 2 \quad (9-2)$$

The doublet r_5, x_5 may now be found and an interpolation between the properties at points 7 and 9 yield the estimate of the flow properties at 5. This information is used to improve the estimate of α_3 in Equation (9-2). The process is continued until convergence is reached. The physical characteristic line passing through point 5 terminates at the shock at point 3. If the compatibility equation is now solved along this line a measure of the inaccuracy of the shock slope will result. Using all the known information concerning points 5 and 3 solve for the flow angle at 3.

$$\bar{\theta}_3^{(n)} = \theta_5^{(n)} - \delta_i Q \left(q_3^{(n)} - q_5^{(n)} \right) + \delta_i G - \delta_i B \quad (9-3)$$

where

$$Q = \frac{\cot \bar{\mu}}{\bar{q}}$$

$$G = \sigma \frac{\sin \bar{\theta} F}{\bar{r}}$$

$$B = \frac{\sin \bar{\mu} \cos \bar{\mu} (s_3 - s_5)}{\bar{R} \bar{r}}$$

$$F = \frac{\sin \bar{\mu} (x_3 - x_5)}{\cos(\bar{\theta} - \delta_1 \bar{\mu})}$$

and, of course, the barred values are averages over the step length.

An error may then be computed;

$$E^{(n)} = \theta_3^{(n)} - \bar{\theta}_3^{(n)}$$

but

$$E^{(n)} = E \left\{ (\theta + \epsilon)_4^{(n)} \right\}$$

and the solution is perturbed until the root is bracketed. The solution is driven to convergence by the method of false position.

It should be pointed out here that the use of linear interpolation is a matter of convenience only. It would be possible, but in general far from practical, to generate by exact means those points which have been approximated.

Section 10

MESH CONSTRUCTION FOR INTERNAL FLOW

The calculations described previously are point or small region solutions. Some process must be defined which successively employs the proper calculation at the proper time in order to describe the entire field. In order to facilitate a description of the mesh construction process let ϕ represent the total knowledge of flow properties at a point in the field. Also let the expression

$$\phi = \psi(\phi_1, \phi_2, \dots, \phi_m)$$

stand for properties at a new point which are computed as a function ψ of (m) other points. There will be basically six such functional operations $\psi_o, \psi_I, \psi_B, \psi_{As}, \psi_s, \psi_{PM}$, which stand for input point, interior point, boundary point, attached shock point, shock, and Prandtl-Meyer points. In addition the superscript (u) will indicate that the operation is to be performed in the presence of an upper boundary while (L) indicates a lower boundary.

Due to the complexity of handling multiple shock waves, a single shock wave restriction will be imposed. This shock wave is arbitrarily chosen to be of the right running family. This type of problem will most frequently occur in cases of interest. If a left running shock wave occurs the problem is simply inverted.

The choice of right running shock waves also dictates that left running characteristic lines be followed in the calculation. This allows one to retain a minimum of information, i.e., a known characteristic line (hereafter referred to as (j)) and a line in the process of being computed (k) .

To begin the problem all necessary boundary conditions must, of course, be supplied. In addition a starting line containing N points which are designated ψ_n ($n = 1, \dots, N$) must be supplied.

Figure 6 illustrates a flow field in which there are no discontinuities and in which the mesh construction is terminated when the region of interest has been computed.

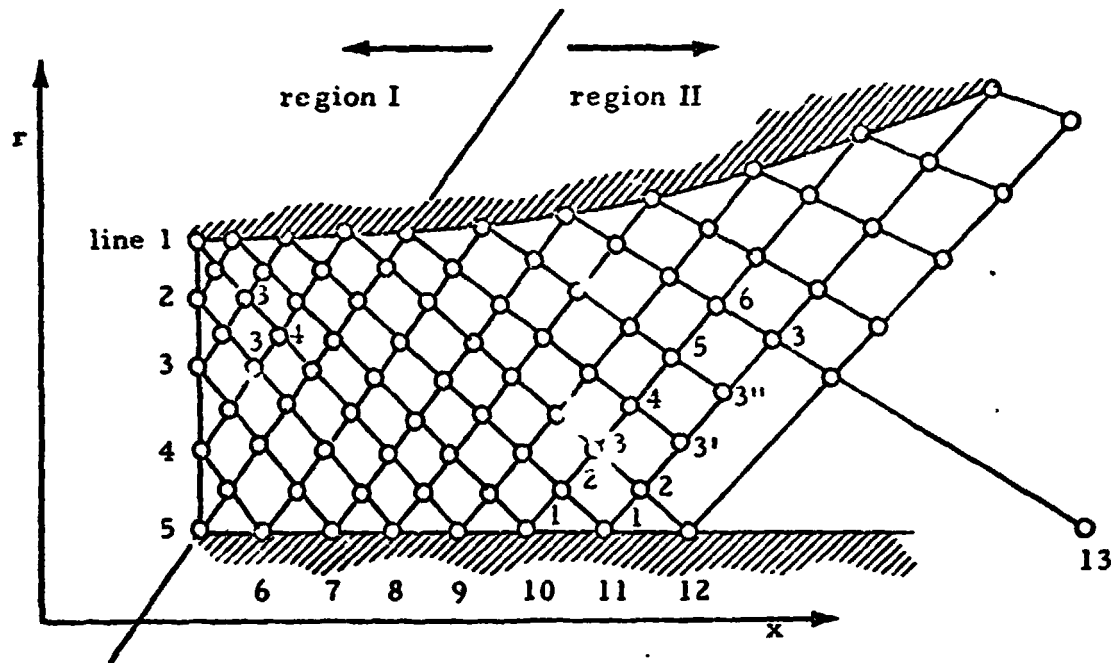


Figure 6

In region I the left running characteristic lines initiate as input points and the mesh construction may be described by;

$$\phi_{i,k} = \begin{cases} \psi_0(\phi_n) & i = 1 \\ \psi_I(\phi_{i-1,k}, \phi_{i-1,j}) & i = 2 \dots (2n-2) \\ \psi_B^u(\phi_{i-1,k}, \phi_{i-2,j}) & i = 2n-1 \end{cases} \quad (10-1)$$

where n varies from 1 to N and $\phi_{i,k}$ represents the flow properties at the i^{th} point on the k line. For instance, in calculating the fourth point on the fourth line shown in the figure, line three is known in its entirety and line four up to and including the third point is known. The above set of relations says that point three on line four and point three on line three will determine, through the interior point solution, the next point (four) on line four.

For region II we have;

$$\phi_{i,k} = \begin{cases} \psi_B^L(\phi_{1,j}, \phi_{2,j}) & i = 1 \\ K_I(\phi_{i-1,k}, \phi_{i+1,j}) & i = 2, \dots, (2N-2) \\ \psi_B^u(\phi_{i-1,k}, \phi_{i,j}) & i = 2N-1 \end{cases} \quad (10-2)$$

As a new line becomes completely defined it may be referred to as j and the process continued indefinitely.

It is possible to combine regions (1) and (2) into a more general scheme if a variable i_N is defined which takes on the value (1) in region I and (0) in region II. At this time the number of points on the j line (i_{T_j}) and the number of points on the new line (i_{T_k}) are defined. Then;

$$\phi_{i,k} = \begin{cases} i_N \psi_0(\phi_n) + (1-i_N) \psi_B^L(\phi_{1,j}, \phi_{2,j}) & i = 1 \\ \left. \begin{matrix} \psi_I(\phi_{ik,k}, \phi_{ij,j}) & \begin{matrix} ik = i-1 \\ ij = i-2i_N+1 \end{matrix} \end{matrix} \right\} & i = 2, \dots, i_{T_k}-1 \\ \left. \begin{matrix} \psi_B^u(\phi_{ik,k}, \phi_{ij,j}) & \begin{matrix} ik = i-1 \\ ij = i-2i_N \end{matrix} \end{matrix} \right\} & i = i_{T_k} \end{cases} \quad (10-3)$$

but

$$i_{T_k} \Leftarrow i_{T_j} + 2i_N$$

Obviously i_{T_j} would have been initialized to (-1) prior to the start of the calculation. When the line is finished i_{T_j} is set to the current value of i_{T_k} .

Thus the process for computing the entire flow field for such a simplified case is described by the set of expressions (10-3). In general, however, discontinuities will arise so that a more flexible description is necessary. If, by some process, points were discarded from the (j) and (k) arrays and the number of points lost is i_{δ_j} and i_{δ_k} respectively then (10-3) becomes;

$$\phi_{i,k} = \begin{cases} i_N \psi_0(\phi_N) + (1-i_N) \psi_B^L(\phi_{1,j}, \phi_{2,j}) & i = 1 \\ \left. \begin{array}{l} \psi_I(\phi_{ik,k}, \phi_{ij,j}) \quad ik = i-1 \\ \quad \quad \quad ij = i-2i_N+1+\tilde{i}_{\delta_j}+\tilde{i}_{\delta_k} \end{array} \right\} & i = 2, \dots, i_{T_k}-1 \\ \left. \begin{array}{l} \psi_B^u(\phi_{ik,k}, \phi_{ij,j}) \quad ik = i-1 \\ \quad \quad \quad ij = i-2i_N+\tilde{i}_{\delta_j}+\tilde{i}_{\delta_k} \end{array} \right\} & i = i_{T_k} \end{cases} \quad (10-4)$$

but

$$i_{T_k} \Leftarrow i_{T_j} + 2i_N - i_{\delta_j} - i_{\delta_k}$$

where the tilda over i_{δ_j} and i_{δ_k} indicates that current values are to be used. These variables are reset to zero at the beginning of each new line.

To illustrate this, imagine that points (1) and (2) have been computed on line 11 and that after point(3) had been computed in the normal fashion it was necessary to discard it. The next point to be computed would then be (3'') but if for some reason it was necessary to discard point 5 on the (j) line then the point (3'') would not exist. Therefore a point has been deleted on each line ($\tilde{i}_{\delta_j} = \tilde{i}_{\delta_k} = 1$) and the diagram and the set of equations (4) indicate that point (6) on line (j) and point (2) on line (k) would be used in the computation of (3) on line (k). Also the total number of points would

have decreased correspondingly. Note that discarding points is the same thing as discarding right running characteristic lines.

It is now possible to include a shock wave into the logic scheme. Since it is a mathematical requirement that characteristic lines of the same family as the shock are continuously intercepted by it, the ability to discard points was necessary. If this was the only mechanism for discarding points then the logic process would be;

$$\phi_{i,k} = \left\{ \begin{array}{ll} i_N \psi_0(\phi_n) + (1-i_N) \psi_B^L(\phi_{1,j}, \phi_{2,j}) & i = 1 \\ \psi_I(\phi_{ik,k}, \phi_{ij,j}) & \left. \begin{array}{l} ik = i-1 \\ ij = i-2i_N+1 \end{array} \right\} i = 2, \dots, i_{s_k} \\ \psi_s(\phi_k, \phi_j) & \left. \begin{array}{l} i = i_{s_k} - i\delta_k \\ i = i_{s_k} - i\delta_k + 1 \end{array} \right\} \\ \psi_I(\phi_{ik,k}, \phi_{ij,j}) & \left. \begin{array}{l} ik = i-1 \\ ij = i-2i_N+1+i\delta_k+i\delta_j \end{array} \right\} i = i_{s_k} - i\delta_k + 2, \dots, i_{T_k} - 1 \\ \psi_B^u(\phi_{ik,k}, \phi_{ij,j}) & \left. \begin{array}{l} ik = i-1 \\ ij = i-2i_N+i\delta_k+i\delta_j \end{array} \right\} i = i_{T_k} \end{array} \right. \quad (10-5)$$

where

$$i_{T_k} \Leftarrow i_{T_j} + 2i_N - i\delta_j - i\delta_k$$

and where i_{s_k} is defined in much the same fashion as i_{T_k} , which is;

$$i_{s_k} \Leftarrow i_{s_j} + 2i_N - 1$$

where i_{s_j} is the location of the upstream shock point on the (j) line.

Figure 7 illustrates the mesh construction when a shock wave is present.

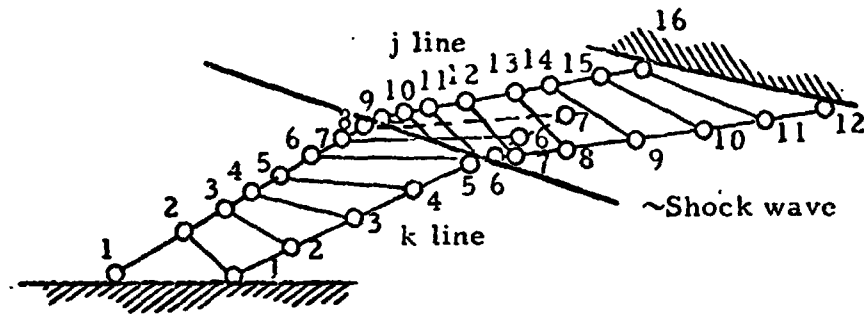


Figure 7

In this example $i_N = 0$ and $i_{s_j} = 8$ so that $i_{s_k} = 7$. Also $i_{T_j} = 16$ so that i_{T_k} would normally also be 16. The (k) line is computed up to point 7 and the shock solution is then employed. In this case the shock solution finds that three points of the (k) line fall downstream of the shock (minimum is one) while two right running lines (points 10 and 11 on the (j) line) also are intercepted by the shock wave. Thus in this example $i_{\delta_k} = 2$ and $i_{\delta_j} = 2$. The set of equations (10-5) then says that the double shock point should be points 5 and 6 on the (k) line and that the total number of points on the (k) line has decreased to 12. Note also that the value of i_{s_j} to begin the next line must be change to 5.

So far no mention of how the shock wave begins has been made. There are two types of shock waves considered; the attached shock wave

which arises due to the flow being forced to negotiate a compression corner on the upper boundary, and the envelope shock. The first of these is easily detected from the boundary conditions and is initially of finite strength. The second type is detected by a mathematical discontinuity in the mesh construction (crossing of right running lines) and is initially of zero strength i.e., a Mach wave. An example of the compression corner solution is given in Figure 8.

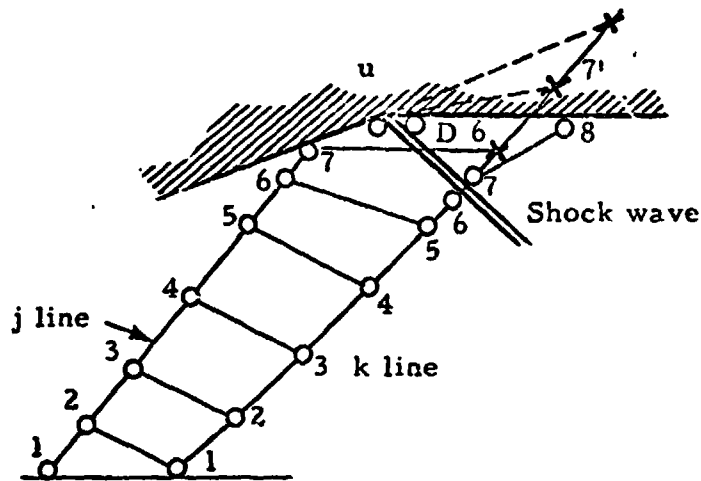


Figure 8

The computation of the (k) line is completed without any prior knowledge that a compression corner exists. A check is made after the boundary solution and the boundary information indicates that a compression corner must be treated. A linear interpolation is performed between the boundary point on line (j) and the fictitious boundary point on line (k) in order to determine the flow properties at point u. An oblique shock calculation is made where the turning angle is known. Using this point and point 6 ($i_{T_k} - 1$) a new virtual point ($\bar{7}$) is computed. i_{s_k} is set to i_{T_k} and the shock solution illustrated in Figure (5e) of Section 6 is employed. This

shock solution completes the (k) line in the proper fashion. In this example $i_{T_j} = 6$ and the next line is computed as previously discussed.

The envelope shock is detected by a crossing of right running characteristic lines as shown in the figure below.

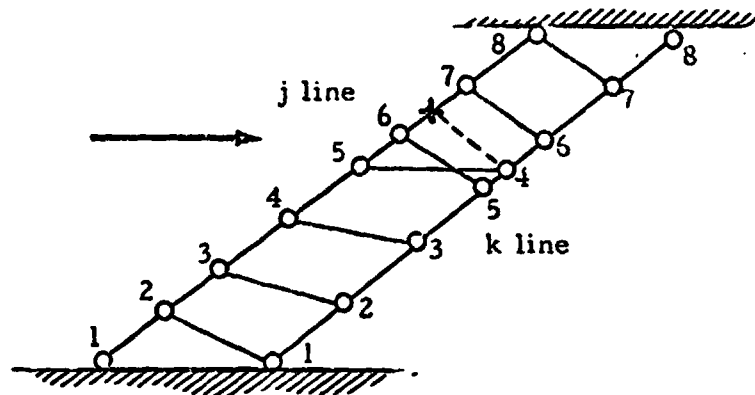


Figure 9

In this example point (5) on the (k) line is found to fall in a previously described region (the region between points (3) and (4) on the (k) line). This discontinuity in the solution is interpreted as a shock wave. If the grid size were chosen small enough the shock wave would initially be of zero strength. Point (5) on line (j) is chosen to be a point which lies on the shock wave and the shock solution is employed. The results of this solution are stored in the normal fashion on the (k) line. Obviously the only difference between this situation and treatment of a previously developed shock wave is to modify the (j) line such that it appears to the logic scheme as though a shock wave crossed the (j) line at point (5).

When an expansion corner is encountered on the upper boundary the

logic scheme is modified locally. Figure 10 illustrates the mesh construction in the vicinity of such a corner.

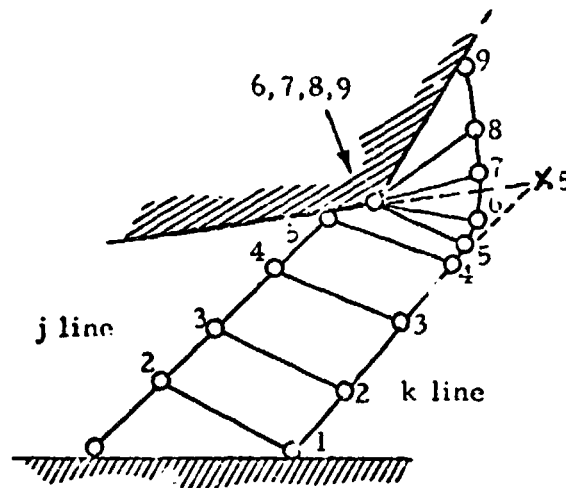


Figure 10

In this case point (5) on line (k) is expected to be a boundary point. It is discovered however, that an expansion corner must be negotiated by the (k) line. A point (6) on the (j) line is found by interpolation. A Prandtl-Meyer calculation is employed and the fan of points is stored in the (j) line above (6). The total number of points to be expected on the (k) line is increased accordingly and the normal logic scheme will now complete the new line. The next line is calculated in the standard fashion.

An expansion corner on a lower wall is somewhat a more complicated situation. Since the calculation no longer utilizes the input line, the lower wall expansion fan may be stored in this area. The set of relations, Equation (10-5) is modified to that of Equation (10-6).

$$\phi_{ij} = \left\{ \begin{array}{l} i_N \psi_0 + (1-i_N) \psi_B^L(\phi_{i,j}, \phi_{2,j}) \\ \psi_I(\phi_{ik,k}, \phi_{ij,j}) \quad \begin{array}{l} ik = i-1 \\ ij = i + (i_\ell - 2) i_N + 1 \end{array} \\ \psi_S(\phi_k, \phi_j) \quad \begin{array}{l} i = i_{s_k} - i_{\delta_k} \\ i = i_{s_k} - i_{\delta_k} + 1 \end{array} \\ \psi_I(\phi_{ik,k}, \phi_{ij,j}) \quad \begin{array}{l} ik = i-1 \\ ij = i + (i_\ell - 2) i_N + i_{\delta_k} + i_{\delta_j} \end{array} \\ \psi_B^u(\phi_{ik,k}, \phi_{ij,j}) \quad \begin{array}{l} ik = i-1 \\ ij = i + (i_\ell - 2) i_N + i_{\delta_k} + i_{\delta_j} \end{array} \end{array} \right\} \quad \begin{array}{l} i = 2, \dots, i_{s_k} \\ i = i_{s_k} - i_{\delta_k} + 2, \dots, i_{T_k} - 1 \\ i = i_{T_k} \end{array}$$

where

$$i_{T_k} \Leftarrow i_{T_j} + (2-i_\ell) i_N - i_{\delta_j} - i_{\delta_k}$$

and where

$$i_{s_k} \Leftarrow i_{s_j} + (2-i_\ell) i_N - 1$$

for which $i_\ell = i_N = 1$ until all fan points are used up.

Section 11 NON-ISOENERGETIC FLOW TREATMENT

The bulk of this document is concerned with the discussion of the analysis of isoenergetic supersonic flow fields. A computer program was written to perform the necessary calculations. Subsequently the computer program was modified to permit the treatment of non-isoenergetic flowfields. Although this treatment is straightforward, decisions were made in the form of the equations and coding of the original program which were not the most advantageous approach when the non-isoenergetic flow situation was considered. In particular, the compatibility equation (6-15) would have been written in the pressure rather than the velocity form. In considering the non-isoenergetic analysis the most expedient way of modifying the computer program was chosen. The development leading to the modified program (consistent with the constraint of minimal impact on the coding rather than straightforwardness of analysis) is presented in this section.

To begin, the development of the species continuity (starting with equation 2-1) could be replaced by atomic conservation equations. Moreover if the conservation of those atoms associated with the fuel and the oxidizer were considered then, for steady state,

$$\nabla \cdot (\rho_f \bar{q}) = 0 \quad (11-1)$$

and

$$\nabla \cdot (\rho_o \bar{q}) = 0 \quad (11-2)$$

would result.

If the weight flow ratio of oxidizer to fuel (O/F ratio) is denoted by η then (11-1) and (11-2) are satisfied if,

$$\bar{q} \cdot \nabla \eta = 0 \quad (11-3)$$

and

$$\nabla \cdot (\rho \bar{q}) = 0 \quad (11-4)$$

The assumptions inherent in arriving at equation (2-40) did not involve isoenergetic flow so that the momentum equation remains valid. The energy equation (2-41), however, remains valid only along a streamline and must be replaced by

$$h + 1/2 \bar{q}^2 = h_o(\eta) \quad (11-5)$$

The equations of Section 3 are modified in an obvious fashion while Section 4 remains unchanged. In Section 5, however, a new variable is introduced into the thermochemistry determination. Since the discussion of Section 5 is pertinent to a single O/F ratio, the gas properties description must be expanded to include a variable O/F. To do this the discussion of Section 5 may be followed for each of two values of the O/F ratio which bracket the desired O/F and a linear interpolation used to generate the required information.

In Section 6 equations (6-1) and (6-2) are valid but now

$$P = P(\rho, s, \eta) \quad \text{so that}$$

$$\nabla P = \left(\frac{\partial P}{\partial \rho} \right)_{s, \eta} \nabla \rho + \left(\frac{\partial P}{\partial s} \right)_{\rho, \eta} \nabla s + \left(\frac{\partial P}{\partial \eta} \right)_{\rho, s} \nabla \eta \quad (11-6)$$

Expanding (11-4) and combining with (11-6) still yields (6-7) since $\bar{q} \cdot \nabla s = \dot{q} \eta = 0$. In equation (6-7), however, it is understood that $a^2 = (\partial P / \partial \rho)_{s, \eta}$.

The definition of γ culminating in equation (6-8) is similarly qualified. Since (6-9) is generated by expansion of (6-7) it remains valid as do all the steps culminating in equation (6-12).

To proceed beyond this point a deviation from the previous approach is taken. Expanding the momentum equation (6-2) results in

$$\frac{1}{\rho} \frac{\partial P}{\partial x} + q \frac{\partial q}{\partial x} = v \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right) \quad (11-7)$$

$$\frac{1}{\rho} \frac{\partial P}{\partial r} + q \frac{\partial q}{\partial r} = -u \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right) \quad (11-8)$$

but from the chain rule

$$\frac{\partial}{\partial n} = \frac{\partial}{\partial x} \frac{\partial x}{\partial n} + \frac{\partial}{\partial r} \frac{\partial r}{\partial n}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial}{\partial r} \frac{\partial r}{\partial t}$$

where (n, t) are respectively normal and tangential to the streamline. Hence,

$$\frac{\partial x}{\partial n} = -\frac{v}{q}, \quad \frac{\partial r}{\partial n} = \frac{u}{q}$$

It then follows that

$$\frac{1}{\rho} \frac{\partial P}{\partial n} + q \frac{\partial q}{\partial n} = -q \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right)$$

and that

$$\frac{\partial v}{\partial x} = \frac{\partial u}{\partial r} - \frac{1}{q} \left(\frac{1}{\rho} \frac{\partial P}{\partial n} + q \frac{\partial q}{\partial n} \right) \quad (11-9)$$

Notice that the last term in (11-9) replaces

$$\frac{a^2}{\gamma R q} \frac{\partial s}{\partial n}$$

in the previous derivation. Following the previous derivation with this in mind the counterpart of (6-15) is easily shown to be

$$d\theta \pm \frac{\cot \mu}{q} \mp \frac{\sin \mu \cos \mu}{\gamma R T} \left(\frac{dP}{\rho} + q dq \right) \mp \frac{\sin \mu \sin \theta}{\sin(\theta \mp \mu)} \frac{\sigma}{r} dr = 0 \quad (11-10)$$

The above result is the compatibility equation used in the isoenergetic flow analysis. Notice that by continued manipulation the pressure form of the compatibility equation will result. That this form of the equation is unaltered by the non-isoenergetic analysis is not surprising since it is constructed entirely based on the momentum equation and the global continuity equation (neither of which are altered by the non-isoenergetic flow phenomena).

The numerical solution to the governing equations is not greatly affected by the modification to the compatibility equation. In equation (6-18)

$$\Delta s_{1,2} \Leftarrow -\frac{1}{T_{1,2}} \left(\frac{\Delta P_{1,2}}{\bar{\rho}_{1,2}} + \bar{q}_{1,2} \Delta q_{1,2} \right) \quad (11-11)$$

while in (6, 25)

$$(s_3 - s_{1,2}) \Leftarrow \frac{1}{T_{1,2}} \left(\frac{\Delta P_{1,2}}{\bar{\rho}_{1,2}} + \bar{q}_{1,2} \Delta q_{1,2} \right) \quad (11-12)$$

Now equations (6-26), (6-27), (6-28) are the finite difference analog to the streamline equation. In a similar fashion we may write